

Drude and Superfluid Weights in Extended Systems: the Role of Discontinuities and δ -peaks in the One and Two-Body Momentum Densities

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Abstract

The question of conductivity is revisited. Using the total momentum shift operator to construct the perturbed many-body Hamiltonian and ground state wave function the second derivative of the ground state energy with respect to the perturbing field is expressed in terms of the one and two-body momentum densities. The distinction between the adiabatic and envelope function derivatives, hence

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that between the Drude and superfluid weights can be introduced in a straightforward manner. It is shown that a discontinuity in the momentum density leads to a contribution to the Drude weight, but not the superfluid weight, however a δ -function contribution in the two-body momentum density (such as in the BCS wave-function) contributes to both quantities. The connection between the discontinuity in the momentum density and localization is also demonstrated.

To distinguish between conductors and insulators an expression for the frequency-dependent conductivity was derived by Kohn [1]. The DC conductivity (Drude weight) corresponds to the strength of the δ -function peak of the conductivity at zero frequency. The Drude weight is often expressed [1, 2] in terms of the second derivative of the ground state energy with respect to a phase associated with the perturbing field. This phase has the effect of shifting the momenta of the system. Scalapino, White, and Zhang (SWZ) [3, 4] have pointed out that taking the derivative with respect to the phase is ambiguous: if the derivative is defined via adiabatically shifting the state which is the ground state at zero field, then the Drude weight results. In the presence of level crossings the adiabatically shifted state may be an excited state for finite perturbation. The superfluid weight is obtained if the derivative corresponds to the “envelope function”, i.e. the ground state for any value of the perturbation. SWZ also state that nonadiabatic crossings occur infinitesimally close to zero field if the dimensionality is greater than one.

In this paper this question is revisited. Based on the total momentum shift operator [5] the perturbed Hamiltonian and ground state wavefunction are explicitly constructed. This operator plays an important role in constructing the total position operator for many-body systems [5, 6, 7]. The second derivative of the ground state energy with respect to the perturbing field is then expressed in terms of the one and two-body momentum densities. It is then shown that the adiabatic and envelope derivatives can be distinguished by varying the length scale associated with the total momentum shift operator, which is also the length scale of the perturbing field. When this length scale is assumed to be the same as the size of the system then $\frac{\partial^2 E(\Phi)}{\partial \Phi^2}$ is proportional to the superfluid weight, if this length scale is assumed to be much larger than the system size then $\frac{\partial^2 E(\Phi)}{\partial \Phi^2}$ corresponds to the Drude weight. For continuous one and two-body momentum densities both quantities are zero. If the one-body momentum density is discontinuous then the Drude weight is finite, but the superfluid weight is zero, and if the two-body momentum displays a δ -peak (Cooper pairing) then both the Drude and superfluid weights are finite. Hence insulators, metals, and superconductors can be distinguished. While a discontinuous momentum density

being a sign of conduction is a well-known result of many-body theory [8] and plays an important role in the Landau theory of Fermi liquids [8, 9], the foundations of the latter are distinct from those for the conductivity put forth by Kohn [1]. In this work the finiteness of the Drude weight and the discontinuity in the momentum density are shown to coincide. Moreover, it is also demonstrated that the localization tenet suggested by Kohn [1], namely that a system localized(delocalized) in the many-body configuration space is insulating(metallic), is also equivalent to the absence(presence) of a discontinuity in the momentum density. Hence the Landau theory of Fermi liquids and the localization theory of Kohn are placed on the same theoretical footing.

We consider a system of interacting fermions whose Hamiltonian is periodic in L . We will assume that the ground state is also periodic in L (i.e. $\Phi = 0$). This leads to no loss of generality, since if the ground state is at a finite Φ , the Hamiltonian can be shifted. We wish to write the Hamiltonian for such a system. We first write

$$\hat{\mathcal{H}} = \mathcal{H}(\{g(k)\}; \{\hat{c}_k^{(\dagger)}\}) \quad (1)$$

where $g(k)$ are continuous functions of k and $\hat{c}_k^{(\dagger)}$ denote creation and annihilation operators of particles at wave-vector k . This Hamiltonian includes only states which are periodic in L . Due to the periodicity the spacing of the points on which the momenta are represented is $\Delta k = 2\pi/L$. $\hat{\mathcal{H}}$ is not the full Hamiltonian of the system, since the states with twisted boundary conditions (which correspond to k -vectors which fall between the grid-points) do not appear as eigenstates. To include them we write

$$\hat{\mathcal{H}}(\alpha) = \mathcal{H}(\{g(k + \alpha)\}; \{\hat{c}_{k+\alpha}^{(\dagger)}\}). \quad (2)$$

Here all the k vectors have been shifted by α , however, the spacing of the k -vectors is unchanged. The full Hamiltonian can be written

$$\hat{\mathcal{H}}_T = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\alpha \hat{\mathcal{H}}(\alpha). \quad (3)$$

This Hamiltonian is the full Hamiltonian in the sense that the system itself is periodic in L , however states of all boundary twists are included. $\hat{\mathcal{H}}_T$ is block-diagonal, since Hamiltonians with different values of α correspond to different Hilbert spaces. In the limit $L \rightarrow \infty$ $\hat{\mathcal{H}}_T$ becomes the full Hamiltonian of the infinite system.

To stress this point one can consider the Hubbard model for a system with size L with Hamiltonian written in reciprocal space,

$$\hat{H}_{Hub} = \sum_{k\sigma} \epsilon_{k\sigma} n_{k\sigma} + U \sum_{kk'q} \hat{c}_{k\uparrow}^\dagger \hat{c}_{k'\downarrow}^\dagger \hat{c}_{k+q\uparrow} \hat{c}_{k'-q\downarrow}. \quad (4)$$

The eigenstates of this Hamiltonian are periodic in L . The spacing of the k -vectors is $\Delta k = 2\pi/L$. The shifted Hubbard Hamiltonian

$$\hat{H}_{Hub} = \sum_{k\sigma} \epsilon_{k+\alpha\sigma} n_{k+\alpha\sigma} + U \sum_{kk'q} \hat{c}_{k+\alpha\uparrow}^\dagger \hat{c}_{k'+\alpha\downarrow}^\dagger \hat{c}_{k+q+\alpha\uparrow} \hat{c}_{k'-q+\alpha\downarrow}, \quad (5)$$

has eigenstates with twisted boundary conditions, however, the Hamiltonian still corresponds to a system periodic in L , as the spacing between the k -vectors is still $\Delta k = 2\pi/L$.

It is expedient to introduce the total momentum shift operator

$$\hat{U}\left(\frac{2\pi}{L}\right) = \exp\left(i\frac{2\pi\hat{X}}{L}\right), \quad (6)$$

where $\hat{X} = \sum_i i\hat{n}_i$, the sum of the positions of all the particles, and which has the property that [5]

$$\hat{U}\left(\frac{2\pi}{L}\right) \hat{c}_k = \begin{cases} \hat{c}_{k-\frac{2\pi}{L}} \hat{U}, & k = 2\frac{2\pi}{L}, \dots, 2\pi \\ \hat{c}_{2\pi} \hat{U}, & k = \frac{2\pi}{L}. \end{cases} \quad (7)$$

We extend $\hat{U}(2\pi/L)$ to lengths nL with n integer. Then momentum shifts to states with twisted boundary conditions on L are also included. Taking the limit $n \rightarrow \infty$ we can write

$$\hat{U}(\gamma) \hat{\mathcal{H}}(\alpha) \hat{U}(-\gamma) = \mathcal{H}(\{g(k+\alpha)\}; \{\hat{c}_{k+\alpha-\gamma}^{(\dagger)}\}), \quad (8)$$

for arbitrary γ thus

$$\hat{U}(\gamma) \hat{\mathcal{H}}_T \hat{U}(-\gamma) = \frac{1}{2\pi} \int_{-\pi}^{\pi} d\alpha \mathcal{H}(\{g(k+\alpha+\gamma)\}; \{\hat{c}_{k+\alpha}^{(\dagger)}\}). \quad (9)$$

The transformed Hamiltonian defined in Eq. (9) has the same eigensystem as $\hat{\mathcal{H}}_T$. The transformation merely shifts the block diagonal Hamiltonians which comprise $\hat{\mathcal{H}}_T$.

The linear response of a system with periodic boundary conditions can be cast using the total momentum shift. We assume that the system of interest has a Hamiltonian of the form

$$\hat{H} = \sum_k \epsilon_k \hat{n}_k + \hat{H}_i, \quad (10)$$

where \hat{H}_i denotes an interaction diagonal in the coordinate representation. This Hamiltonian includes the ground state, which is also periodic in L . For the ground state wavefunction we assume the form,

$$|\Psi(0)\rangle = \sum_{k_1, \dots, k_N} \psi(k_1, \dots, k_N) c_{k_1}^\dagger \dots c_{k_N}^\dagger |0\rangle, \quad (11)$$

which is the most general for fixed particle number.

The usual way to introduce a static vector potential $A\hat{x}$ is to multiply the hopping parameters with a phase factor. In this case the k vectors are shifted as $k \rightarrow k + \Phi$ with $\Phi = A/\hbar c$, leading to

$$\hat{H}(\Phi) = \sum_k \epsilon_{k+\Phi} \hat{n}_k + \hat{H}_i. \quad (12)$$

To arrive at Eq. (12) one can also use the total momentum shift operator on the total Hamiltonian constructed from \hat{H} , and shift indices as was done to obtain Eq. (9). In the same way one can obtain the wavefunction corresponding to the shifted $\hat{H}(\Phi)$,

$$|\Psi(\Phi)\rangle = \sum_{k_1, \dots, k_N} \psi(k_1 + \Phi, \dots, k_N + \Phi) c_{k_1}^\dagger \dots c_{k_N}^\dagger |0\rangle. \quad (13)$$

The criterion for the DC conductivity and the superfluid weight can both be written [2, 3, 4] in the form

$$D = \frac{1}{2L} \frac{d^2 E(0)}{d\Phi^2}. \quad (14)$$

While the Drude weight and the superfluid weight quantities correspond to different perturbations, the expression for these quantities coincides, since in the above expression $\Phi = 0$, hence the explicit dependence on the vector potential, which gives rise to the distinction, is neglected. Taking advantage of the Hellmann-Feynman theorem D can be expressed as

$$D = \frac{1}{2L} \left\{ \langle \Psi(0) | \frac{\partial^2 H(0)}{\partial \Phi^2} | \Psi(0) \rangle + \langle \frac{\partial \Psi(0)}{\partial \Phi} | \frac{\partial H(0)}{\partial \Phi} | \Psi(0) \rangle + \langle \Psi(0) | \frac{\partial H(0)}{\partial \Phi} | \frac{\partial \Psi(0)}{\partial \Phi} \rangle \right\}. \quad (15)$$

The reason that both the Drude and superfluid weights can be written in this form is due to the fact that Eq. (15) is a linear response expression in which the effect of the perturbing field is set to zero.

The derivatives with respect to Φ of the Hamiltonian can be made to correspond with derivatives with respect to the momenta, i.e. it holds that,

$$\frac{\partial \hat{H}(\Phi)}{\partial \Phi} = \sum_k \frac{\partial \epsilon_{k+\Phi}}{\partial k} \hat{n}_k, \quad (16)$$

and

$$\frac{\partial^2 \hat{H}(\Phi)}{\partial \Phi^2} = \sum_k \frac{\partial^2 \epsilon_{k+\Phi}}{\partial k^2} \hat{n}_k, \quad (17)$$

$$\frac{\partial|\Psi(\Phi)\rangle}{\partial\Phi} = \sum_{k_1, \dots, k_N} \sum_i \frac{\partial\psi(k_1 + \Phi, \dots, k_N + \Phi)}{\partial k_i} c_{k_1}^\dagger \dots c_{k_N}^\dagger |0\rangle. \quad (18)$$

The derivative with respect to k is ambiguous [3, 4]. For a finite system with size L the summation in Eqs. (16), (17), and (18) is defined on grid points separated by $2\pi/L$ in reciprocal space. Thus one way to define the derivatives is using these grid points (for example the finite element definition).

The total momentum shift extended to length nL extends the Hilbert space, hence the derivatives can also be defined using the extended states on the finer grid $2\pi/(nL)$. Note that the summations in Eqs. (16), (17), and (18) are still defined on the grid $2\pi/L$. When the thermodynamic limit is taken ϵ_k is a continuous function, hence this distinction between grids causes no ambiguity in the application of Eqs. (16) and (17). The wavefunction, however, can be discontinuous, and, as discussed below, this leads to consequences. Using Eqs. (16), (17), and (18) one can show that

$$D = \frac{1}{2L} \sum_k \left(\frac{\partial^2 \epsilon_k}{\partial k^2} n_k + \frac{\partial \epsilon_k}{\partial k} \left(\frac{\partial n_k}{\partial k} + \sum_{k'} \frac{\partial n_{k,k'}^{(2)}}{\partial k'} \right) \right), \quad (19)$$

where n_k and $n_{k,k'}^{(2)}$ denote the one and two-body momentum densities in the ground state, defined as

$$n_k = \sum_i \sum_{\substack{k_1, \dots, k_N \\ k_i = k}} |\psi(k_1, \dots, k_N)|^2 \quad (20)$$

and

$$n_{k,k'}^{(2)} = \sum_{i \neq j} \sum_{\substack{k_1, \dots, k_N \\ k_i = k, k_j = k'}} |\psi(k_1, \dots, k_N)|^2. \quad (21)$$

Eq. (19) is arrived at by using Eqs. (16), (17), and (18), and the identity

$$\langle 0 | \hat{c}_{k_N} \dots \hat{c}_{k_1} \hat{n}_k \hat{c}_{k_1}^\dagger \dots \hat{c}_{k_N}^\dagger | 0 \rangle = \sum_i \delta_{k_i k}. \quad (22)$$

For the case $n = 1$, we replace the derivative in Eq. (19) by

$$\frac{\partial n_k}{\partial k} \rightarrow \frac{n_{k+2\pi/L} - n_k}{2\pi/L}. \quad (23)$$

This definition corresponds to the “envelope function” definition of SWZ [3, 4]. To see this consider the system at $\Phi = 0$ and $\Phi = 2\pi/L$. The ground state at $\Phi = 0$ is of the form in Eq. (11), at $\Phi = 2\pi/L$ it is Eq. (13), no longer the ground state in general. For both $\Phi = 0$ and $\Phi = 2\pi/L$ the ground

state density is given by n_k . In Eq. (23) the function n_k (corresponding to the ground state) is used in both cases. When the thermodynamic limit ($L \rightarrow \infty$) is taken the first two terms in Eq. (19) cancel due to partial integration resulting in

$$D^{(n=1)} = \frac{L}{8\pi^2} \int dk dk' \frac{\partial \epsilon_k}{\partial k} \frac{\partial n_{k,k'}^{(2)}}{\partial k'}. \quad (24)$$

This quantity integrates to zero, due to the periodicity of the Brillouin zone, unless, as discussed below, pairing occurs in the two-body density. These arguments allow association of $D^{(n=1)}$ with the superfluid weight.

We now consider the implications of the different properties of the derivatives for $n = 1$ and $n \rightarrow \infty$. For segments for which n_k and $n_{k,k'}^{(2)}$ are continuous the two definitions of the derivatives (based on the spacing $2\pi/L$ vs. $2\pi/(nL)$) coincide, however this is not true when either densities are discontinuous in k . While on the larger grid $2\pi/L$ a discontinuity in these quantities leads to a divergence, on the grid $2\pi/(nL)$ the discontinuity does not occur when the derivative at the k -grid points is evaluated and the limit $n \rightarrow \infty$ is taken first, and the derivative is defined as adiabatically shifted.

As an example one can consider a Fermi sea, for which the term depending on the two-body density does not contribute since there are no correlations between momenta. When a phase is applied the energy levels and the momentum densities are shifted as $\epsilon_k \rightarrow \epsilon_{k+\Phi}$, $n_k \rightarrow n_{k+\Phi}$. If the phase $\Phi \approx 2\pi/L$, and the ground state of the new Hamiltonian is used in defining the derivative (“envelope function”), then the discontinuity *contributes* to the derivative, since if n_k is the last filled state near the discontinuity, then $n_{k+2\pi/L}$ will be the first unfilled one. However, for small Φ (which corresponds to the limit $n \rightarrow \infty$) if n_k corresponds to the last filled state then $n_{k+\Phi}$ does not change. Excluding the discontinuities (which are relevant to the second term in Eq. (19)) from the partial integral leads to

$$D^{(n \rightarrow \infty)} = \frac{1}{2\pi} \Delta n_{k_F} \frac{\partial \epsilon_{k_F}}{\partial k}, \quad (25)$$

where the discontinuities are assumed to be at $k = \pm k_F$ (Fermi wave vector). When spin is included then each spin component will contribute a term of the form in Eq. (25). For this reason we associate the quantity $D^{(n \rightarrow \infty)}$ with the Drude weight.

To explore the connection between conduction and the discontinuity in the momentum density further we consider the quantity

$$\Pi(y) = \left| \langle \Psi | \hat{U}(y) | \Psi \rangle \right| = \left| \sum_{k_1, \dots, k_N} \psi^*(k_1 + y, \dots, k_N + y) \psi(k_1, \dots, k_N) \right|. \quad (26)$$

The quantity $(L^2/(2\pi^2)\text{Re } \ln \Pi(2\pi/L))$ was suggested by Resta and Sorella as a criterion of localization. As a result of Kohn's hypothesis [1] localization is also a criterion to distinguish conductors from insulators. If the wavefunction $\psi(k_1, \dots, k_N)$ is a continuous functions of its arguments then $\Pi(2\pi/L)$ approaches unity in the limit of large system size. The functions n_k and $\Pi(y)$ are then continuous, corresponding to insulation. When n_k is discontinuous then the magnitude of the wavefunction $\psi(k_1, \dots, k_N)$ is also discontinuous. In the following we assume that the magnitude of $\psi(k_1, \dots, k_N)$ is discontinuous but its phase is not. Since $\psi(k_1, \dots, k_N)$ describes indistinguishable particles, the discontinuity has to occur as a function of any of its arguments. Moreover, on physical grounds we anticipate that this discontinuity occurs at the Fermi wave-vector. The effect of the discontinuity can be assessed by considering the difference

$$\begin{aligned} \Pi(0) - \Pi(\epsilon) = & \left| \frac{1}{(2\pi)^N} \int dk_1 \dots dk_N \psi^*(k_1, \dots, k_N) \psi(k_1, \dots, k_N) \right| \\ & - \left| \frac{1}{(2\pi)^N} \int dk_1 \dots dk_N \psi^*(k_1 + \epsilon, \dots, k_N + \epsilon) \psi(k_1, \dots, k_N) \right|. \end{aligned} \quad (27)$$

where ϵ denotes an infinitesimal and the thermodynamic limit was taken. The integrands in the first term and the second term will cancel for regions where the coefficient $\psi(k_1, \dots, k_N)$ is continuous. The contribution of a discontinuity at k_F will be of the form

$$\rho(k_F+; k_F+) + \rho(k_F-; k_F-) - \rho(k_F+; k_F-) - \rho(k_F-; k_F+), \quad (28)$$

where $\rho(k; k')$ denotes the one-body density matrix in k -space. Rewriting in a natural orbital representation this contribution takes the form

$$\sum_i q_i [\gamma_i^*(k_F+) \gamma_i(k_F+) + \gamma_i^*(k_F-) \gamma_i(k_F-) - \gamma_i^*(k_F+) \gamma_i(k_F-) - \gamma_i^*(k_F-) \gamma_i(k_F+)], \quad (29)$$

(with $0 \leq q_i \leq 1$ and $\gamma_i(k)$ denoting the natural orbitals) which under the assumption of a continuous phase is a positive quantity. Since this is also the case for $\Pi(0) - \Pi(-\epsilon)$ it follows that for discontinuous coefficient $\psi(k_1, \dots, k_N)$ the function $\Pi(y)$ will contain a δ -function contribution at the origin. These results coincide exactly with the results of Resta and Sorella [7] where a function of the quantity $|\Pi(2\pi/L)|$ is suggested as a criterion of localization and conduction.

To understand the effect of pairing we study the BCS wavefunction

$$|\Psi_{BCS}\rangle = \prod_k (u_k + v_k c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger) |0\rangle. \quad (30)$$

We assume a BCS Hamiltonian with constant coupling between Cooper pairs. Calculating the properties of this wavefunction requires generalization to

include spin and variable particle number of Eq. (19) which presents no difficulty. Since the one-body density of the BCS wavefunction is continuous the first two terms cancel by partial integration when the thermodynamic limit is taken. Thus we are lead to consider the last term only, which depends on the two-body momentum density $n_{k,k'}^{(2)}$. This quantity can be broken up into components with parallel and anti-parallel spins. The parallel spin two-body density is again continuous, hence does not contribute. The two-body density when the spins are anti-parallel gives

$$n_{k,k'}^{(2)} = \begin{cases} f(k') & k' = -k \\ f(k)f(k') & k' \neq -k, \end{cases} \quad (31)$$

with

$$f(k) = \frac{|v_k|^2}{|u_k|^2 + |v_k|^2}. \quad (32)$$

Explicit calculation for the BCS wavefunction then yields for the thermodynamic limit

$$D = \frac{1}{4\pi} \sum_{\sigma} \int dk \left(-\frac{\partial \epsilon_k}{\partial k} \frac{\partial n_{k\sigma}}{\partial k} \right) + \frac{L}{8\pi^2} \sum_{\sigma} \int dk dk' \frac{\partial \epsilon_k}{\partial k} n_{k\sigma} \frac{\partial n_{k'-\sigma}}{\partial k}.$$

The first term arises since $n_{k\sigma, -k-\sigma}^{(2)} = n_{k\sigma}$, i.e. due to Cooper pairing. Due to the continuity of $n_{k\sigma}$ the last term is zero. Partial integration then results in

$$D = \frac{1}{4\pi} \sum_{\sigma} \int dk \frac{\partial^2 \epsilon_k}{\partial k^2} n_{k\sigma}. \quad (33)$$

Since the function $f(k)$ is continuous this result holds for both $n = 1$ and $n \rightarrow \infty$. The result that the second derivative of the “envelope” function of the ground state energy is finite for a superfluid and zero for a normal metal was obtained for the case of a ring with finite thickness by Byers and Yang [10].

SWZ have also shown [4] that for dimensions higher than one the first non-adiabatic crossing occurs at zero field when the thermodynamic limit is taken. This leads to a distinction between evaluating $\frac{\partial^2 E(\Phi)}{\partial \Phi^2}$ first and then taking the thermodynamic limit or vice versa. In generalizing the formalism presented here to higher dimensions one has to consider that the differential operators in the superfluid and Drude weights operate in one particular direction (that of the perturbing field). If the thermodynamic limit is first taken in the direction perpendicular to the perturbing field, then the discontinuity can “disappear”. For example, a two-dimensional non-interacting system at half-filling has a discontinuous momentum density, n_{k_x, k_y} , but the function

$f(k_x) = \int dk_y n_{k_x, k_y}$ is a continuous function. However, the definition of the derivative corresponding to the case $n \rightarrow \infty$ resolves this ambiguity. In that case irrespective of the order of limits the discontinuity will be excluded from the integration, as argued above for the Fermi sea. Moreover, as shown above, the discontinuity in the momentum density contains exactly the same information as the localization order parameter of Resta and Sorella [7], a quantity which is also insensitive to dimensionality.

In conclusion the second derivative of the ground state energy with respect to a perturbing field (vector potential) at zero field was derived and shown to be an expectation value over the one and two-body momentum densities. A length scale associated with the perturbation was defined, and through it states with twisted boundary conditions were introduced, allowing for the possibility of defining the adiabatic derivative (Drude weight) and the derivative of the ground state energy envelope function (superfluid weight). The resulting expression for the Drude weight is not the zero frequency limit of an quantity based on time-dependent perturbation theory. The Drude weight is finite in the presence of discontinuities in the wavefunction (which correspond to discontinuities in the momentum densities), as well as due to BCS pairing. The superfluid weight is not sensitive to discontinuities in the momentum densities, but is finite in the presence of BCS pairing. It was shown that a localization quantity suggested by Resta and Sorella [7] based on a tenet of Kohn [1] contains the same information as the discontinuity in the momentum density. Thus the connection between the localization hypothesis of Kohn [1] and the criterion of metallicity in the Landau theory of Fermi liquids is established.

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